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KINETICS OF FORMIC ACID AT HIGH PRESSURE AND TEMPERATURE*

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Abstract

We have developed a detailed kinetic model to follow the decomposition of formic acid at modestly high pressures (1-10 GPa) and temperature (500-1000K) and further include our refinement of a fluid exponential-6 equation of state for formic acid and corresponding reaction species. We also include the effects of bimolecular and water catalyzed reactions, calculated from *ab initio* molecular orbital calculations. We present a comparison between our simulations and experimental observations made using near-simultaneous high-pressure FTIR and Raman spectroscopy. We discuss, in detail, the implications our experimental observations provide in relation to computed reaction timescales and dominant species employed in our model.

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